

Theoretical Study of Interplay Between Superconductivity and Itinerant Ferromagnetism

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Abstract: Following Green's function technique and equation of motion method, the coexistence of superconductivity (SC) and itinerant ferromagnetism (FM) is investigated in a single band homogenous system. Self consistent equations for SC and FM order parameters, Δ and m or I respectively are derived. It is shown that there generally exists a coexistent ($\Delta \neq 0$, and m or $I \neq 0$) solutions to the coupled equations of the order parameter in the temperature range $0 < T < \min(T_C, T_{FM})$, where T_C and T_{FM} are respectively the superconducting and ferromagnetic transition temperatures. Expressions for specific heat, density of states, free energy and critical field are derived. The specific heat has linear temperature dependence as opposed to the exponential decrease in the BCS theory. The density of states for a finite m increases as opposed to that of a ferromagnetic metal. Free energy study reveals that FM-SC state has lowest energy than the normal FM state and therefore realized at low enough temperature. Effect of small external field is also studied. The theory is applied to explain the observations in uranium based intermetallics systems *UCoGe* and *UIr*. The agreement between theory and experiments is quite encouraging.

Keywords: Itinerant ferromagnetism, Green's function, Superconductivity, Energy spectra and density of states, BCS Hamiltonian, Hubbard Hamiltonian.

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1. INTRODUCTION

The recent discovery the coexistence of superconductivity (SC) and itinerant ferromagnetism (FM) in Uranium based intermetallics compounds: UGe_2 [1], URhGe [2], UIr [3] and UCoGe [4] have attracted a great interest and revived the interest in the old problem of coexistence of superconductivity and ferromagnetism [5-9]. In these Uranium intermetallics magnetism has a strong itinerant character and both ordering phenomena are carried by the same 5f electrons. The experiments indicate that in these materials:

- (i) The superconducting phase is completely covered within the ferromagnetic phase and disappears in the paramagnetic phase.
- (ii) The ferromagnetic order is stable within the superconducting phase.
- (iii) The specific heat anomaly associated with the superconductivity in these materials appears to be absent. The specific heat depends on the temperature linearly at low temperature [10].

Numerous theoretical studies have tried to answer the question what the attractive forces are between the electrons leading to the formation of Cooper pairs [11-32]. The general features of the proposed models are:

- (i) The superconducting pairing of the conduction electrons is mediated by spin fluctuations rather than by phonons, as is the case in conventional superconductors.
- (ii) In the superconducting state quasiparticles form Cooper pairs in which the spins are parallel ($S = 1$) in contrast to conventional superconductors with opposite spin ($S = 0$).
- (iii) The ferromagnetism is itinerant and therefore carried by the conduction electrons. This arises from a splitting of the spin-up and spin-down band. A consequence is that the ferromagnetism and superconductivity is carried by same electrons.

Early theories proposed magnetically mediated spin – triplet superconductivity [27]. Suhl [19], Zhou and Gong [24], Mineev and Champel [17] have also favoured magnetically mediated spin – triplet superconductivity in these systems. Following Suhl's work [19], Abrikosov [20] have shown that this mechanism can lead only to an s – wave order parameter. Superconductivity appears together with ferromagnetism but persists only until the ferromagnetism is weak. Watanabe and Miyake [13] are of the opinion that the superconductivity in these systems is mediated by the coupled charge density wave (CDW) and spin density wave (SDW) fluctuations originating from the CDW ordering of the majority - spin band.

Powell et al. [25] have considered spin singlet and spin triplet states with either equal spin pairing (ESP) or opposite spin pairing (OSP) states. They found that gap equations for the singlet state reproduced the Clogston – Chandrasekhar limiting behaviour [33,34] and the phase diagram of the Baltensperger – Sarma equation [35,36]. They also showed that the singlet gap equation leads to the result that the superconducting order parameter is independent of exchange splitting at zero temperature. They further found that OSP triplet states showed a very similar behaviour to the singlet state in the presence of exchange splitting. Blagoev et al. [26] have studied the problem in terms of diagrammatic many – body theory, on the basis of the itinerant electron model. Machida and Ohmi [11] have given arguments for the pairing to be of p – wave, normally spin – triplet nature. It is not obvious from these considerations why the superconductivity is observed only in the ferromagnetic phase. To explain this Sandeman et al. [14] proposed a density of states effect that exists only in the ferromagnetic phase, as the source of the superconductivity in UGe₂. Kirkpatrick et al. [15,16] proposed an explanation for the observed phase diagram that is based on an enhancement of the longitudinal spin susceptibility in the ferromagnetic phase by magnons or magnetic Goldstone modes. Most theories which describe ferromagnet close to a quantum phase transition have predicated that the superconducting transition temperature, T_c , should be at least as high in the paramagnetic state as it is in the ferromagnetic state. These theories have considered an electronically three – dimensional ferromagnet, either magnetically isotropic [21] or uniaxial [23].

Kirkpatrick et al [15,16] have predicated an enhancement of the superconducting transition temperature T_c in the ferromagnetic regime from the coupling of magnons to the longitudinal magnetic susceptibility. However, the ferromagnetic state of these systems is highly anisotropic – at 4.2 K and an external magnetic field of 4T, the easy – axis magnetization is 20 to 30 times that along either of the other crystallographic axes [37] – so transverse modes seem unlikely to explain the exclusively ferromagnetic superconductivity in these systems.

Gorski et al. [38] have studied the possibility of simultaneous coexistence of superconductivity and ferromagnetism within the framework of the extended Hubbard model. The main driving forces for these phenomena considered by these authors are kinetic interactions. They reported that even weak ferromagnetism, if generated by the band shift, destroys the superconductivity. The ferromagnetism created by a change of bandwidth can coexist with the singlet superconductivity. However, it seems difficult to understand the simultaneous coexistence of superconductivity and ferromagnetism in these

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systems in terms of these theories and require a novel concept to understand : (i) how the same band electrons are responsible for both the superconductivity and ferromagnetism, and (ii) why the superconductivity occurs only in the ferromagnetic phase, i.e. what is the microscopic relationship between these two antagonistic phenomena?

The theories of itinerant ferromagnetic superconductors stated above provide a basic understanding of the new phenomenon in these systems, but a microscopic theory and a satisfactory mechanism seems still lacking.

In the present paper, we propose a simple microscopic theory of ferromagnetic superconductors which explain satisfactorily the observed features of these systems and also predict the qualitative behaviour of energy spectra and density of states function $N(\omega)$, superconducting order parameter (Δ), magnetic order parameter (m), electronic specific heat, free energy , critical field and effect of small external field. In this class of materials, UIr holds a special place because it is a system in which the crystal structure lacks inversion symmetry.

2. THE MODEL HAMILTONIAN

We propose the following model Hamiltonian:

$$H = H_0 + H_{\text{BCS}} + H_H \quad (1)$$

with

$$H_0 = \sum_{K,\sigma} \{ \epsilon_\sigma(K) - \mu \} C_{K\sigma}^+ C_{K\sigma} \quad (2)$$

where

$$\epsilon_\sigma(K) = \{ \epsilon(K) - \mu_B h \sigma \} \quad (3)$$

$$\sigma = \begin{cases} 1 & \text{for the spin up} \\ -1 & \text{for the spin down} \end{cases}$$

$h (= \mu_0 H)$ is small external field in tesla. $C_{K\sigma}^+$ ($C_{K\sigma}$) are the fermion creation (annihilation) operators for the Bloch states, $|\mathbf{K}, \sigma\rangle$, where \mathbf{K} is the conduction electron wave vector and σ is its spin. $\epsilon(K)$ is the single electron energy in the f-band and measured from the bottom of the band and μ is the chemical potential. The operators $C_{K\sigma}^+, C_{K\sigma}$ satisfy the usual fermion anti – commutation rules.

$$H_{\text{BCS}} = -\Delta \sum_K (C_{-K\downarrow} C_{K\uparrow} + C_{K\uparrow}^+ C_{-K\downarrow}^+) \quad (4)$$

is the BCS Hamiltonian [39]. Δ is superconducting order parameter and is chosen real and positive. Δ is only a weak function of \mathbf{K} and therefore we have neglected its \mathbf{K} dependence. Δ is determined self – consistently from the gap equation

$$\Delta = \frac{|g|}{N} \sum_{\mathbf{K}} \langle C_{\mathbf{K}\uparrow}^+ C_{-\mathbf{K}\downarrow}^+ \rangle \quad (5)$$

$|g|$ ($|g| > 0$) is the phonon – mediated electron – electron coupling constant having the dimensions of energy. The summation over \mathbf{K} is limited by the wave vector corresponding to Debye's energy $\hbar\omega_D$ at the Fermi surface. $\langle \dots \rangle$ indicates the thermodynamic average.

$$H_H = \frac{U}{N} \sum_{\mathbf{K}, \mathbf{K}'} C_{\mathbf{K}\uparrow}^+ C_{\mathbf{K}\downarrow}^+ C_{\mathbf{K}\downarrow} C_{\mathbf{K}\uparrow} \quad (6)$$

is the Hubbard Hamiltonian [40]. U is the repulsive Coulomb interaction, which is responsible for the ferromagnetic transition.

Combining equations (2), (4) and (6), the model Hamiltonian (1) can be expressed in the following mathematical form.

$$H = \sum_{\mathbf{K}, \sigma} \{ \epsilon_{\mathbf{K}} - \mu - \mu_B \hbar \sigma \} C_{\mathbf{K}\sigma}^+ C_{\mathbf{K}\sigma} - \Delta \sum_{\mathbf{K}} (C_{-\mathbf{K}\downarrow} C_{\mathbf{K}\uparrow} + C_{\mathbf{K}\uparrow}^+ C_{-\mathbf{K}\downarrow}^+) + \frac{U}{N} \sum_{\mathbf{K}, \mathbf{K}'} C_{\mathbf{K}\uparrow}^+ C_{\mathbf{K}'\downarrow}^+ C_{\mathbf{K}'\downarrow} C_{\mathbf{K}\uparrow} \quad (7)$$

We define

$$n_{\sigma} = \frac{1}{N} \sum_{\mathbf{K}} \langle C_{\mathbf{K}\sigma}^+ C_{\mathbf{K}\sigma} \rangle \quad (8)$$

and use the following notations.

$$n = n_{\uparrow} + n_{\downarrow} = \left(C_{\uparrow}^+ C_{\uparrow} + C_{\downarrow}^+ C_{\downarrow} \right) \quad (9)$$

$$m = n_{\uparrow} - n_{\downarrow} = \left(C_{\uparrow}^+ C_{\uparrow} - C_{\downarrow}^+ C_{\downarrow} \right) \quad (10)$$

$$n_{\sigma} = \frac{n}{2} + \frac{m\sigma}{2} \quad (\sigma = \pm 1) \quad (11)$$

Where n is the total number of electrons per unit cell, μ_B is Bohr magneton and μ_0 is magnetic permeability of free space. It is proposed to solve the Hamiltonian (7) with the help of Green's function technique using the equation of motion method.

2.1 GREEN'S FUNCTIONS

In order to study the physical properties of itinerant ferromagnetic superconductors, we define electron Green's functions for the conduction band electrons which are subjected to the ferromagnetic and superconducting instability. The electron Green's functions are defined in the usual way as follows:

$$\begin{aligned} G_{\uparrow\uparrow}(\mathbf{K}'', \mathbf{K}', t) &= \langle\langle C_{\mathbf{K}''\uparrow}; C_{\mathbf{K}'\uparrow}^+ \rangle\rangle_{\omega} \\ &= -i\theta(t) \langle [C_{\mathbf{K}''\uparrow}(t), C_{\mathbf{K}'\uparrow}^+(0)] \rangle \end{aligned} \quad (12)$$

$$\begin{aligned} G_{\downarrow\downarrow}(\mathbf{K}'', \mathbf{K}', t) &= \langle\langle C_{\mathbf{K}''\downarrow}; C_{\mathbf{K}'\downarrow}^+ \rangle\rangle_{\omega} \\ &= -i\theta(t) \langle [C_{\mathbf{K}''\downarrow}(t), C_{\mathbf{K}'\downarrow}^+(0)] \rangle \end{aligned} \quad (13)$$

$$\begin{aligned} F_{\uparrow\uparrow}^+(\mathbf{K}'', \mathbf{K}', t) &= \langle\langle C_{-\mathbf{K}''\downarrow}^+; C_{\mathbf{K}'\uparrow}^+ \rangle\rangle_{\omega} \\ &= i\theta(t) \langle [C_{-\mathbf{K}''\downarrow}^+(t), C_{\mathbf{K}'\uparrow}^+(0)] \rangle \end{aligned} \quad (14)$$

$$\begin{aligned} F_{\uparrow\downarrow}(\mathbf{K}'', \mathbf{K}', t) &= \langle\langle C_{-\mathbf{K}''\uparrow}; C_{\mathbf{K}'\downarrow} \rangle\rangle_{\omega} \\ &= -i\theta(t) \langle [C_{-\mathbf{K}''\uparrow}(t), C_{\mathbf{K}'\downarrow}(0)] \rangle \end{aligned} \quad (15)$$

Following equation of motion method, we obtain following expressions for Green's functions,

$$\langle\langle C_{\mathbf{K}\uparrow}, C_{\mathbf{K}\uparrow}^+ \rangle\rangle = \frac{\delta_{\mathbf{K}\mathbf{K}'} [\omega + (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) - Un \uparrow]}{[\{\omega - (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) - Un \downarrow\} \{\omega + (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) - Un \uparrow\} - \Delta^2]} \quad (16)$$

$$\langle\langle C_{\mathbf{K}\downarrow}, C_{\mathbf{K}\downarrow}^+ \rangle\rangle = \frac{\delta_{\mathbf{K}\mathbf{K}'} [\omega + (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) + Un \downarrow]}{[\{\omega + (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) - Un \uparrow\} \{\omega + (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) + Un \downarrow\} - \Delta^2]} \quad (17)$$

$$\langle\langle C_{-\mathbf{K}\downarrow}^+, C_{\mathbf{K}\uparrow}^+ \rangle\rangle = \frac{-\Delta \delta_{\mathbf{K}\mathbf{K}'}}{[\{\omega - (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) - Un \downarrow\} \{\omega + (\epsilon_{\mathbf{K}} - \mu - \mu_{\mathbf{B}} h\sigma) - Un \uparrow\} - \Delta^2]} \quad (18)$$

2.2 CORRELATION FUNCTIONS

Using the relation [5,7,41]

$$\langle B(t')A(t) \rangle = \lim_{\epsilon \rightarrow 0} \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{\langle\langle A(t); B(t') \rangle\rangle_{\omega+i\epsilon} - \langle\langle A(t); B(t') \rangle\rangle_{\omega-i\epsilon}}{e^{B\omega} - 1} \times [\exp[i\omega(t-t')]] d\omega \quad (19)$$

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and employing the identity,

$$\lim_{\epsilon \rightarrow 0} \left(\frac{1}{\omega + i\epsilon - E_K} - \frac{1}{\omega - i\epsilon - E_K} \right) = -2\pi i \delta(\omega - E_K) \quad (20)$$

one obtains the correlation function for the Green's functions given by equations (16) to (18) as

$$\begin{aligned} \langle C_{K\uparrow}^+ C_{K\uparrow} \rangle &= f(\alpha_2) + \frac{\alpha_1}{\alpha_1 - \alpha_2} \{f(\alpha_1) - f(\alpha_2)\} \\ &+ \frac{(\epsilon_K - \mu - \mu_B h\sigma) + Un \downarrow}{\alpha_1 - \alpha_2} \{f(\alpha_1) - f(\alpha_2)\} \end{aligned}$$

or

$$\begin{aligned} \langle C_{K\uparrow}^+ C_{K\uparrow} \rangle &= f(\alpha_2) + \frac{\alpha_1 + (\epsilon_K - \mu - \mu_B h\sigma) + Un \downarrow}{\alpha_1 - \alpha_2} \\ &\times \{f(\alpha_1) - f(\alpha_2)\} \end{aligned} \quad (21)$$

Where

$$\alpha_1 = -\frac{Um}{2} + \sqrt{\Delta^2 + \left\{ (\epsilon_K - \mu - \mu_B h\sigma) + \frac{Un}{2} \right\}^2}$$

And

$$\alpha_2 = -\frac{Um}{2} - \sqrt{\Delta^2 + \left\{ (\epsilon_K - \mu - \mu_B h\sigma) + \frac{Un}{2} \right\}^2} \quad (22)$$

and $f(\alpha_1)$ and $f(\alpha_2)$ are Fermi functions. Similarly, one obtains the other correlation functions as

$$\langle C_{K\downarrow}^+ C_{K\downarrow} \rangle = \frac{\alpha_2' + \alpha_1' + (\epsilon_K - \mu - \mu_B h\sigma) + Un \downarrow}{\alpha_1' - \alpha_2'} \{f(\alpha_1') - f(\alpha_2')\} \quad (23)$$

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where $\alpha_1' = -\alpha_2$ and $\alpha_2' = -\alpha_1$ and $f(\alpha_1')$ and $f(\alpha_2')$ are Fermi functions.

$$\langle C_{-K\uparrow}^+ C_{K\downarrow}^+ \rangle = -\frac{\Delta}{\alpha_1 - \alpha_2} \left[\{f(\alpha_1) - f(\alpha_2)\} \right] \quad (24)$$

Using these Green's functions and correlation functions the expressions for various physical properties of itinerant ferromagnetic superconductors can be derived.

3. PHYSICAL PROPERTIES

3.1 SUPERCONDUCTING ORDER PARAMETER (Δ)

Δ is determined self – consistently from the gap equation

$$\Delta = \frac{|g|}{N} \sum_{\mathbf{K}} \langle C_{K\uparrow}^+ C_{-K\downarrow}^+ \rangle \quad (25)$$

$|g|$ ($|g| > 0$) is the phonon – mediated electron – electron coupling constant having the dimensions of energy. The summation over \mathbf{K} is limited by the wave vector corresponding to Debye's energy $\hbar\omega_D$ at the Fermi surface. $\langle - - - \rangle$ indicates the thermodynamic average. By substituting the correlation function given by equation (24).

$$\begin{aligned} \frac{1}{|g|N(o)} &= \int_{\mu-\hbar\omega_D}^{\mu+\hbar\omega_D} d\epsilon_K \frac{1}{(\alpha_1 - \alpha_2)} \left[\frac{1}{e^{\beta\alpha_2} + 1} - \frac{1}{e^{\beta\alpha_1} + 1} \right] \\ \text{or } \frac{1}{|g|N(o)} &= \int_{\mu-\hbar\omega_D}^{\mu+\hbar\omega_D} d\epsilon_K \frac{1}{4\sqrt{\Delta^2 + \left\{ (\epsilon_K - \mu - \mu_B h\sigma) + \frac{Un}{2} \right\}^2}} \\ &\quad \times \left[\tanh \frac{\beta\alpha_1}{2} - \tanh \frac{\beta\alpha_1}{2} \right] \\ &= \int_0^{\hbar\omega_D} d\epsilon_K \frac{1}{2\sqrt{\Delta^2 + \left\{ (\epsilon_K - \mu_B h\sigma) + \frac{Un}{2} \right\}^2}} \\ &\quad \times \left[\tanh \frac{\beta\alpha_1}{2} - \tanh \frac{\beta\alpha_1}{2} \right] \end{aligned} \quad (26)$$

Where α_1 and α_2 are given by equation (22).

Putting $m = 0$ and $U = 0$ in equation (26), we observe that it reduces to the standard BCS equation [39],

$$\frac{1}{|g|N(0)} = \int_0^{\hbar\omega_D} \frac{dx}{x} \tanh \frac{x}{2k_B T_C} \quad (27)$$

where k_B is Boltzmann constant and T_C is superconducting critical transition temperature.

Analyzing the expression (26), we see that the presence of magnetization reduces the volume of the phase space that is available for the Cooper pair. This leads to the decrease in gap at $T = 0$ and hence T_C will also be reduced compared to the BCS value for given values of other relevant parameters. Obviously, the increase in magnetization pushes the gap away from the Fermi surface and reduces its magnitude also [42]

Equation (26) is the general expression for the superconducting order parameter Δ for itinerant ferromagnetic superconductors.

3.2 MAGNETIZATION (m)

From equation (10), we have –

$$m = n \uparrow - n \downarrow$$

Obviously, the fermions which form Cooper pairs are the same as those responsible for spontaneous magnetization.

Using equation (8), the above relation takes the form.

$$m = \frac{1}{N} \sum_{\mathbf{k}} \langle C_{\mathbf{k}\uparrow}^+ C_{\mathbf{k}\uparrow} \rangle - \frac{1}{N} \sum_{\mathbf{k}} \langle C_{\mathbf{k}\downarrow}^+ C_{\mathbf{k}\downarrow} \rangle \quad (28)$$

Using equations (21 and (23), the equation (28) takes the form.

$$m = \frac{1}{N} \sum_{\mathbf{k}} \left[\frac{1}{e^{\beta E_-} + 1} - \frac{1}{e^{\beta E_+} + 1} \right] \quad (29)$$

where

$$E_- = E_{\mathbf{k}} - I \quad (30)$$

$$E_+ = E_{\mathbf{k}} + I \quad (31)$$

are the quasiparticle energy relations. Here,

$$I = \frac{Um}{2} \quad (32)$$

and

$$E_{\mathbf{k}} = \sqrt{\Delta^2 + \left[(\epsilon_{\mathbf{k}} - \mu - \mu_B h\sigma) + \frac{Un}{2} \right]^2} \quad (33)$$

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Now, one can write the magnetic energy splitting I between the spin – up and spin – down band as

$$I = \frac{Um}{2} = \frac{U}{2N} \sum_K [f(E^-) - f(E^+)] \quad (34)$$

or

$$I = \left(\frac{u}{2}\right) \sum_K [f(E^-) - f(E^+)] \quad (35)$$

where $u = U/N$ and $f(E)$ is Fermi function.

Equation (26) is the BCS gap equation in the presence of a finite magnetization m . Equation (35) is the equation which determines the magnetization when the superconducting state may be present. Here the superconducting gap Δ and the magnetic energy splitting I between the spin-up and spin-down bands are independent order parameters. The system of equations (26) and (34) determines the phase where the superconductivity and ferromagnetism coexist.

The equations (26) and (34) have the following solutions :

- (i) normal or paramagnetic state $\Delta = 0, I = 0$;
- (ii) ferromagnetic state $\Delta = 0, I \neq 0$;
- (iii) superconducting state $\Delta \neq 0, I = 0$; and
- (iv) coexistent state $\Delta \neq 0, I \neq 0$.

From equations (26) and (34), we find that magnetization m and superconducting order parameter Δ have dependencies such as $m = m(g, U, T)$ and $\Delta = \Delta(g, U, T)$. Moreover, they are coupled with each other through the distribution functions, which are also functions of m and Δ . From the numerical solutions of these two coupled equations (26) and (34), we will get the values of m and Δ to be used for the calculation of the physical properties.

The ferromagnetic transition temperature T_{FM} can be obtained from Equation (29). Equation (29) cannot be solved exactly and therefore we evaluate it numerically.

3.3. SPECIFIC HEAT (C^s)

The electronic specific heat per atom of a superconductor is determined from the following relation [6,8,43].

$$C^s = \frac{\partial}{\partial T} \frac{1}{N} \sum_K 2(\epsilon_K - \mu - \mu_B h \sigma) < C_{K\uparrow}^+ C_{K\uparrow} > \quad (36)$$

Changing the summation over \mathbf{K} into integration and substituting the correlation function $\langle C_{\mathbf{K}\uparrow}^+ C_{\mathbf{K}\uparrow} \rangle$, one obtains.

or

$$\begin{aligned} \frac{C^S}{T} = & \frac{2N(o)}{N} \frac{1}{T^2} \int_0^{\hbar\omega_D} d\epsilon_K \left[\frac{\beta\alpha_2 \exp(\beta\alpha_2)}{[\exp(\beta\alpha_2) + 1]^2} \right. \\ & + \frac{\beta(\alpha_1 + \epsilon_K - \mu_B \hbar\sigma + Un \downarrow)(\epsilon_K - \mu_B \sigma \hbar)}{2\sqrt{\Delta^2 + \left\{(\epsilon_K - \mu_B \sigma \hbar) + \frac{Un}{2}\right\}^2}} \\ & \left. \times \left(\frac{\alpha_1 \exp(\beta\alpha_1)}{[\exp(\beta\alpha_1) + 1]^2} - \frac{\alpha_2 \exp(\beta\alpha_2)}{[\exp(\beta\alpha_2) + 1]^2} \right) \right] \end{aligned} \quad (37)$$

One can solve equation (37) numerically for electronic specific heat.

3.4 ENERGY SPECTRA AND DENSITY OF STATES

If we compare the quasiparticle energy spectra given by equations (30) and (31) with the BCS energy spectrum $E = \sqrt{\epsilon_K^2 + \Delta^2}$, we note that the modification is due to the presence of the ferromagnetic energy. We can easily verify that the gap appears not at the Fermi level, rather it is pushed up. Now, the energy spectrum is symmetrical around $E = Um$, contrary to the BCS case where it was symmetric around $E = 0$.

Now, we derive the expressions for the density of states. Density of states is one of the most important function to be determined and the one which is most susceptible to experimental verification as a function of the excitation energy ϵ_K [6-8, 39].

The density of states per atom per spin, $N(\omega)$ is given by [44]

$$N(\omega) = \lim_{\epsilon \rightarrow 0} \frac{i}{2\pi N} \sum_K G_{\uparrow\uparrow}[(K, \omega + i\epsilon) - G_{\uparrow\uparrow}(K, \omega - i\epsilon)] \quad (38)$$

Here $G_{\uparrow\uparrow}(K, \omega)$ is the one particle Green's function given by equation (17). From equations (38) and (17), using following relation:

$$\lim_{\epsilon \rightarrow 0} \left\{ \frac{1}{\omega + i\epsilon - \epsilon_K} - \frac{1}{\omega - i\epsilon - \epsilon_K} \right\} = 2\pi i \delta(\omega - \epsilon_K) \quad (39)$$

we obtain

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$$N(\omega) = N(0) \frac{(\omega + \mu_B h \sigma) + (Um/2)}{\left[\left((\omega + \mu_B h \sigma) + (Um/2) \right)^2 - \Delta^2 \right]^{1/2}} \quad (40)$$

$$\frac{N(\omega)}{N(0)} = \frac{(\omega + \mu_B h \sigma) + I}{\left[\left((\omega + \mu_B h \sigma) + I \right)^2 - \Delta^2 \right]^{1/2}} \quad (41)$$

In the limit $I \rightarrow 0$, equation (41) reduces to

$$\frac{N(\omega)}{N(0)} = \begin{cases} \frac{\omega}{\sqrt{\omega^2 - \Delta^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \quad (42)$$

which is same as described by the BCS theory [39].

The important effect of the magnetization is that it modifies the density of states, which affect the superconducting gap. We evaluate equation (42) numerically for obtaining density of states.

3.5 FREE ENERGY

Alongwith the nonzero solution, describing the coexistence of ferromagnetism and superconductivity, there is a solution of equations (26) and (35) with a vanishing gap describing normal ferromagnetic state. For the transition from the normal ferromagnetic state to the superconducting – ferromagnetic state to take place the energy of the former state must be lower than the energy of the latter state. One can calculate the difference between two energies using the relation [44-53],

$$\frac{F_{SF} - F_{NF}}{V} = \int_0^\Delta d\Delta \Delta^2 \frac{d}{d\Delta} \left(\frac{1}{|g|} \right) \quad (43)$$

This form is particularly convenient because equation (43) expresses $\frac{1}{|g|}$ as a function of Δ (T), and direct substitution leads to

$$\begin{aligned} \frac{F_{SF} - F_{NF}}{V} &= N(0) \int_0^{\hbar\omega_D} d\epsilon \int_0^\Delta d\Delta (\Delta^2) \frac{d}{d\Delta} \left[\frac{1}{(\alpha_1 - \alpha_2)} \left(\frac{1}{e^{B\alpha_2} + 1} - \frac{1}{e^{B\alpha_1} + 1} \right) \right] \quad (44) \\ &= N(0) \int_0^{\hbar\omega_D} d\epsilon \int_0^\Delta d\Delta (\Delta^2) \frac{d}{d\Delta} \left[\frac{1}{(\alpha_1 - \alpha_2)} \left(\tanh \frac{\beta\alpha_1}{2} - \tanh \frac{\beta\alpha_2}{2} \right) \right] \quad (45) \end{aligned}$$

Putting $U = 0$ and $h = 0$ in equation (45), it reduces to standard BCS expression [11],

$$\frac{F_{SF} - F_{NF}}{V} = N(0) \int_0^{\hbar\omega_D} d\epsilon_K \int_0^{\Delta} d\Delta(\Delta^2) \frac{d}{d\Delta} \left\{ \frac{\tanh\left(\frac{1}{2}\beta E\right)}{E} \right\} \quad (46)$$

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Where $E = \sqrt{\Delta^2 + \epsilon_K^2}$

Writing equation (45) as

$$\frac{F_{SF} - F_{NF}}{V} = N(0) \int_0^{\hbar\omega_D} d\epsilon_K \int_0^{\Delta} d\Delta(\Delta^2) \frac{d}{d\Delta} \left\{ \frac{1}{2\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \sigma h + \frac{Un}{2}\right)^2}} \left(\tanh \frac{\beta\alpha_1}{2} - \tanh \frac{\beta\alpha_2}{2} \right) \right\} \quad (47)$$

or

$$\begin{aligned} \frac{F_{SF} - F_{NF}}{V} &= \frac{N(0)}{2} \int_0^{\hbar\omega_D} d\epsilon_K \int_0^{\Delta} d\Delta(\Delta^2) \frac{d}{d\Delta} \left(\frac{1}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h \sigma + \frac{Un}{2}\right)^2}} \tanh \frac{\beta\alpha_1}{2} \right) \\ &\quad - \frac{N(0)}{2} \int_0^{\hbar\omega_D} d\epsilon_K \int_0^{\Delta} d\Delta(\Delta^2) \frac{d}{d\Delta} \left(\frac{1}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h \sigma + \frac{Un}{2}\right)^2}} \tanh \frac{\beta\alpha_2}{2} \right) \\ &= \frac{N(0)}{2} \int_0^{\hbar\omega_D} d\epsilon_K \left(\frac{\Delta^2}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h \sigma + \frac{Un}{2}\right)^2}} \tanh \frac{1}{2} \beta \left\{ \frac{Un}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h \sigma + \frac{Un}{2}\right)^2} \right\} \right) \\ &\quad - \int_0^{\Delta} d\Delta \left(\frac{\Delta}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h \sigma + \frac{Un}{2}\right)^2}} \tanh \frac{\beta\alpha_1}{2} \right) \end{aligned}$$

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$$\begin{aligned}
& -\frac{N(0)}{2} \int_0^{\hbar\omega_D} d\epsilon_K \left[\frac{\Delta^2}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_K \hbar\sigma + \frac{U_N}{2}\right)^2}} \tanh \frac{1}{2} \beta \left\{ \frac{U_M}{2} \sqrt{\Delta^2 + \left(\epsilon_K - \mu_K \hbar\sigma + \frac{U_N}{2}\right)^2} \right\} \right] \\
& + \int_0^{\Delta} d\Delta \left[\frac{\Delta}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_K \hbar\sigma + \frac{U_N}{2}\right)^2}} \tanh \frac{\beta\alpha_1}{2} \right]
\end{aligned} \tag{48}$$

where the second and fourth line is obtained with partial integration. The first and third terms together is just similar to the right side of the BCS gap equation [11],

$$\frac{1}{|g|N(0)} = \int_0^{\hbar\omega_D} \frac{d\epsilon_K}{\left(\epsilon_K^2 + \Delta^2\right)^{1/2}} \tanh \frac{\beta\left(\epsilon_K^2 + \Delta^2\right)^{1/2}}{2} \tag{49}$$

The second and fourth terms can be simplified by changing variables from

$$\Delta \text{ to } t = \sqrt{\Delta^2 + \left(\epsilon_K + \mu_B \hbar\sigma + \frac{U_N}{2}\right)^2}. \text{ In this way, one obtains}$$

$$\begin{aligned}
\frac{F_{SF} - F_{NF}}{V} &= \frac{N(0)\Delta^2}{2} \int_0^{\hbar\omega_D} d\epsilon_K \left[\frac{1}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{U_N}{2}\right)^2}} \tanh \left(\frac{1}{2} \beta \alpha_1 \right) \right] \\
& - \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\epsilon_K \ell n \left[\frac{\cosh \frac{\beta}{2} \left[-\frac{U_M}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{U_N}{2}\right)^2} \right]}{\cosh \frac{\beta}{2} \left[-\frac{U_M}{2} + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{U_N}{2}\right) \right]} \right]
\end{aligned}$$

$$\begin{aligned}
& -\frac{N(0)\Delta^2}{2} \int_0^{\hbar\omega_D} \left[\frac{d\epsilon_K}{\sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2}\right)^2}} \tanh\left(\frac{1}{2}\beta\alpha_2\right) \right] + \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\epsilon_K \\
& \quad \ln \left\{ \frac{\cosh\frac{\beta}{2} \left[-\frac{Um}{2} - \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2}\right)^2} \right]}{\cosh\frac{\beta}{2} \left[-\frac{Um}{2} - \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2}\right) \right]} \right\} \\
& = \frac{\Delta^2}{g} - \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\epsilon_K \left[\ln \left(1 + e^{\left[-\beta \left(-\frac{Um}{2} + \sqrt{\Delta^2 + \left(\epsilon_K + \mu_B \hbar\sigma + \frac{Un}{2}\right)^2} \right)} \right) \right. \right. \\
& \quad \left. \left. + \frac{1}{2}\beta \left(-\frac{Um}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2}\right)^2} - \left\{ \frac{Um}{2} + \epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2} \right\} \right) \right] \right. \\
& \quad \left. + \frac{4N(0)}{2} \int_0^{\hbar\omega_D} d\epsilon_K \ln \left[1 + \exp \left\{ -\beta \left(-\frac{Um}{2} + \epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2} \right) \right\} \right] \right. \\
& \quad \left. - \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\epsilon_K \ln \left[1 + \exp \left\{ -\beta \left(-\frac{Um}{2} - \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2}\right)^2} \right) \right\} \right] \right. \\
& \quad \left. + \frac{1}{2}\beta \left(-\frac{Um}{2} - \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2}\right)^2} - \left\{ \frac{Um}{2} - \epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2} \right\} \right) \right] \right. \\
& \quad \left. + \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\epsilon_K \ln \left(1 + e^{\left[-\beta \left\{ \frac{Um}{2} - \epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2} \right\} \right]} \right) \right]
\end{aligned}$$

Since $\hbar\omega_D \gg k_B T$, the second and fourth integrals on the right may be extended to infinity. An easy calculation then shows that it equals the first temperature – dependent correction to the thermodynamic potential in the normal ferromagnetic state [11]. We have

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$$\frac{4N(o)V}{\beta} \int_0^\infty d\epsilon_K \left[\ln \left(1 + e^{-\beta \left\{ \frac{Um}{2} + \epsilon_K - \mu_B \sigma h + \frac{Un}{2} \right\}} \right) \right] \quad (51)$$

$$= \frac{1}{3} N(0) V \pi^2 (k_B T)^2$$

$$\approx [F_{NF}(T) - F_{NF}(0)]$$

In addition, it is readily verified that [11]

$$\begin{aligned} & -2N(0) \int_0^{\hbar\omega_D} d\epsilon_K \left[\left(-\frac{Um}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2} \right)^2} \right) - (\epsilon_K - \mu_B \sigma h) \right] \\ & \approx -N(0) \left(\frac{1}{2} \Delta^2 + \Delta^2 \ln \frac{2\hbar\omega_D}{\Delta} \right) \end{aligned} \quad (52)$$

$$= -\frac{1}{2} N(0) \Delta^2 - \frac{\Delta^2}{g} - N(0) \Delta^2 \ln \frac{\Delta_0}{\Delta}$$

After simplification, one obtains the expression for free energy difference between superconducting – ferromagnetic state and normal ferromagnetic state as

$$\begin{aligned} \frac{F_{SF} - F_{NF}}{V} &= -\frac{1}{2} N(0) \Delta^2 - N(0) \Delta^2 \ln \left(\frac{\Delta_0}{\Delta} \right) \\ & - 4N(0) k_B T \int_0^{\hbar\omega_D} d\epsilon_K \ln \left(1 + e^{-\beta \left\{ -\frac{Um}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B \hbar\sigma + \frac{Un}{2} \right)^2} \right\}} \right) \\ & + \frac{1}{3} \pi^2 N(0) (k_B T)^2 \end{aligned} \quad (53)$$

Where Δ_0 is the zero temperature gap, whose value can be determined from

$$\beta \Delta_0 = \pi e^{-\gamma} = 1.76 \quad (54)$$

which is a universal constant independent of the particular material.

On further simplification, equation (53) finally takes the form

$$\begin{aligned} \frac{F_{\text{SF}} - F_{\text{NF}}}{V} = & -\frac{1}{2} N(0) \Delta^2 - N(0) \Delta^2 \ln \left(\frac{\Delta_0}{\Delta} \right) \\ & - 4N(0) k_B T \int_0^{\hbar \omega_D} d\epsilon_K \ln \left[1 + e^{-\beta \left\{ -\frac{U\mathbf{m}}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h\sigma + \frac{U\mathbf{n}}{2} \right)^2} \right\}} \right] \\ & + \frac{1}{3} \pi^2 N(0) (k_B T)^2 \end{aligned} \quad (55)$$

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This shows that the superconducting ferromagnetic state has lower energy than the normal ferromagnetic state and therefore will be realized at low enough temperature [39,54]., we evaluate numerically equation (55) for free energy.

3.6 LOW TEMPERATURE CRITICAL FIELD (H_c)

The critical field H_c (T) called the thermodynamic field for the transition between the normal ferromagnetic to superconducting ferromagnetic state is given by the difference of free energies [46].

$$\frac{H_c^2}{8\pi} = -F_{\text{SF}} - F_{\text{NF}} \quad (56)$$

A combination with equation (55), equation (56) yield

$$\begin{aligned} H_c = & (8\pi V)^{1/2} \left[-\frac{1}{2} N(0) \Delta^2 - N(0) \Delta^2 \ln \left(\frac{\Delta_0}{\Delta} \right) - \frac{4N(0)}{\beta} \int_0^{\hbar \omega_D} d\epsilon_K \ln \right. \\ & \left. \times \left\{ 1 + \exp \left[-\beta \left\{ -\frac{U\mathbf{m}}{2} + \sqrt{\Delta^2 + \left(\epsilon_K - \mu_B h\sigma + \frac{U\mathbf{n}}{2} \right)^2} \right\} \right] \right\} \right] + \frac{1}{3} \pi^2 \frac{N(0)}{\beta^2} \end{aligned} \quad (57)$$

In the limit $U \rightarrow 0$ and $h \rightarrow 0$, equation (57) gives the low temperature critical field as

$$\begin{aligned} H_c(T) = & \left[4\pi N(0) \Delta_0^2 \right]^{1/2} \left[1 - \frac{e^{2\gamma}}{3} \left(\frac{T}{T_c} \right)^2 \right] \\ \approx & H_c(0) \left[1 - 1.06 \left(\frac{T}{T_c} \right)^2 \right] T \rightarrow 0 \end{aligned} \quad (58)$$

where

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$$H_c(0) = [4\pi N(0)\Delta_0^2]^{1/2} \quad (59)$$

is the critical field at $T = 0$. One can solve numerically equation (57) to get the behaviour of critical field.

4. NUMERICAL CALCULATIONS

4.1 Superconducting and Magnetic order parameters

Expression (26) is the expression from which we can study the variation of superconducting order parameter with temperature for ferromagnetic superconductors. Using the values of parameters given in tables 1 and 2 for UCoGe and UIr and solving numerically, we obtain values of Δ at various

Table 1: Values of Various Parameters for the System UCoGe

Parameter	Value	References
* Crystal Structure	Orthorhombic TiNiSi structure a = 6.845 Å b = 4.206 Å, c = 7.222 Å Space group P_{nma}	68,69
* Curie temperature (T_{FM})	3 K	4,59,70-71
* Superconducting transition temperature (T_c)	0.8 K	4,59,70-71
* Electronic Specific heat coefficient (γ)	0.057 J K ⁻² mol ⁻¹	72
* Phonon energy ($\hbar\omega_D$)	1.7×10^{-21} J	9,73-75
* Repulsive Coulomb energy U	0.169×10^{-19} J	9,73-75
* Number of electrons per unit cell (n)	4	68
* Magnetization per atom	$\cong 0.7 \times 10^{-2}$	74
* Magnetic energy splitting $\left(I = \frac{Um}{2} \right)$ between spin up and spin down bands	$\cong 1.92 \times 10^{-21}$ J/atom	74
* BCS attractive interaction strength g	3.8×10^{-19} J/atom	73-75
* Density of States at the Fermi Surface, $N(0)$	$\cong 0.24 \times 10^{19}$ per Joule per atom	73-75
Fermi Wave Vector, K	1.62 Å^{-1}	73-75

Table 2: Values of Various Parameters for the System UIr			Theoretical Study of Interplay Between Superconductivity and Itinerant Ferromagnetism
Parameter	Value	References	
• Crystal structure	Monoclinic PbBi type structure (space group P2 ₁) a = 5.62 Å, b = 10.59 Å, c = 5.60 Å,	3	
• Superconducting Transition Temperature (T _c).	0.14 K	3	
• Curie Temperature (T _{FM}) (with low–temperature ordered moment)	46 K at ambient pressure	75,76	
• Electronic specific heat coefficient (γ)	0.049 J K ⁻² mol ⁻¹	3	
• Phonon energy (ħω _D)	1.68 × 10 ⁻²¹ J	9,73-75	
• Repulsive Coulomb energy U	0.158 × 10 ⁻¹⁹ J	9,73-75	
• Density of States at the Fermi Surface (N(0))	0.22 × 10 ¹⁹ per Joule per atom	9,73-75	
• BCS attractive interaction strength g	3.9 × 10 ⁻¹⁹ J/ atom	9,73-75	
• Number of electrons per unit cell (n)	8	9,73-75	
• Magnetization per atom (m)	≅ 0.71 × 10 ⁻²	74	
• Fermi wave vector, K	1.62 Å ⁻¹	9,73-75	
• Magnetic energy splitting $\left(I = \frac{Um}{2} \right)$	1.68 × 10 ⁻²¹ J/ atom	4,75,76	
between spin up and spin down bands			

temperatures below T_c as shown in Table 3 and 4 and variation is shown in figs. 1 and 2 respectively. From these graphs, we note that

- (i) Superconducting transition temperature for UCoGe and UIr are 0.8 K and 0.14 K respectively.
- (ii) Δ versus T variation is just similar to BCS.
- (iii) In comparison to BCS value of T_c (T_c^{BCS}), T_c for ferromagnetic superconductors is slightly lower, i.e. magnetization suppresses superconductivity. This result is in agreement with Karchev [10,55], Karchev et al. [56] and Linder and Sudbo [54].

Table 3: Superconducting order parameter (Δ) for UCoGe

Temperature (T) K	Superconducting order parameter $\Delta = x \times 10^{-21} \text{ J}$		
	Theory	$h = 0.4 \text{ T}$	BCS
0.000	2.20	2.05	2.50
0.100	2.19	2.04	2.49
0.150	2.17	2.02	2.48
0.200	2.14	2.00	2.46
0.270	2.09	1.95	2.41
0.320	2.04	1.90	2.37
0.420	1.91	1.74	2.25
0.520	1.72	1.51	2.10
0.620	1.40	1.15	1.86
0.720	0.86	0.45	1.49
0.750	0.62	0.00	1.34
0.780	0.30	-	1.15
0.800	0.00	-	1.00
0.850	-	-	0.55
0.900	-	-	0.00

- (iv) Effect of small external field ($h = 0.4 \text{ T}$) is also studied on superconductivity. We observe from figs. 1 and 2 that small external field suppresses superconductivity.

4.2 Magnetization

Expression (29) is the expression from which we can study the variation of magnetization (m) with temperature for ferromagnetic superconductors. Using the values of various parameters given in tables 1 and 2 for UCoGe and UIr and solving numerically, we obtain values of m at different temperature as given in tables 5 and 6 and the variation of m with T as shown in figs. 3 and 4 respectively. From these graphs, we note that

- (i) Curie temperature for UCoGe and UIr is 3K and 46 K respectively.

In addition to the solutions described above, we have solved equations (26) and (34) for the coexistent state ($\Delta \neq 0, I \neq 0$). Values of Δ and I within

Table 4: Superconducting order parameter (Δ) for UIr

Temperature (T) K	Superconducting order parameter $\Delta = x \times 10^{-21} \text{ J}$		
	Theory	$h = 0.4 \text{ T}$	BCS
0.000	1.400	1.250	1.700
0.010	1.400	1.240	1.700
0.020	1.400	1.230	1.690
0.030	1.380	1.200	1.676
0.040	1.350	1.160	1.651
0.050	1.301	1.094	1.614
0.060	1.247	1.018	1.553
0.070	1.160	0.924	1.486
0.080	1.072	0.806	1.393
0.090	0.960	0.676	1.300
0.100	0.819	0.520	1.180
0.110	0.640	0.350	1.050
0.120	0.452	0.165	0.880
0.130	0.235	0.000	0.680
0.140	0.000	-	0.470
0.150	-	-	0.230
0.160	-	-	0.000

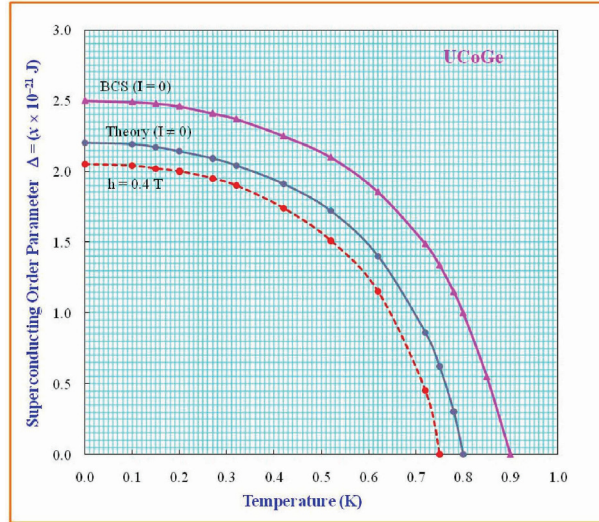


Figure 1: Variation of superconducting order parameter (Δ) with temperature (T) for UCoGe. For $I = 0$, BCS curve is shown.

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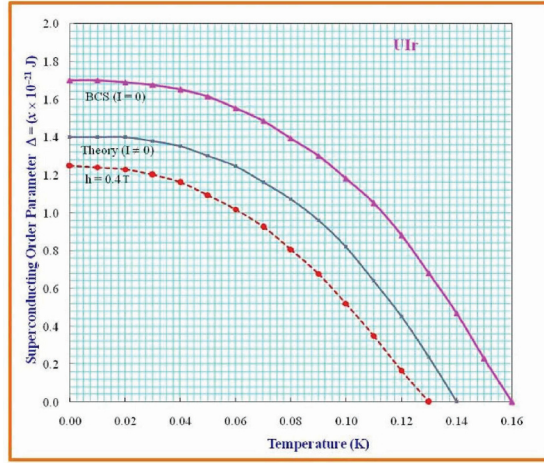


Figure 2: Variation of superconducting order parameter (Δ) with temperature (T) for UIr. For $I = 0$, and $h = 0$, BCS curve is shown.

Table 5: Magnetization (m) for UCoGe

Temperature (T)	Magnetization m (T)
K	
0.000	1.9900
0.300	1.9740
0.500	1.9550
0.700	1.9400
1.000	1.9000
1.200	1.8600
1.500	1.7700
1.700	1.6920
2.000	1.5580
2.300	1.3530
2.600	0.9740
2.800	0.5960
3.000	0.0000

the coexistent state for UCoGe are given in table 7 and behaviour of Δ and I is shown in fig. 5. The behaviour of Δ and I in the coexistence region for UCoGe is quite unusual.

Analysis of the expression (29) shows that the presence of magnetization reduces the volume of the phase space that is available for the Cooper

Table 6: Magnetization (m) for UIr

Temperature (T)	Magnetic order parameter
K	m (T)
0.0	1.750
5.0	1.740
10.5	1.720
16.8	1.650
24.1	1.520
29.5	1.349
33.2	1.200
37.0	1.000
40.5	0.700
45.0	0.190
46.0	0.000

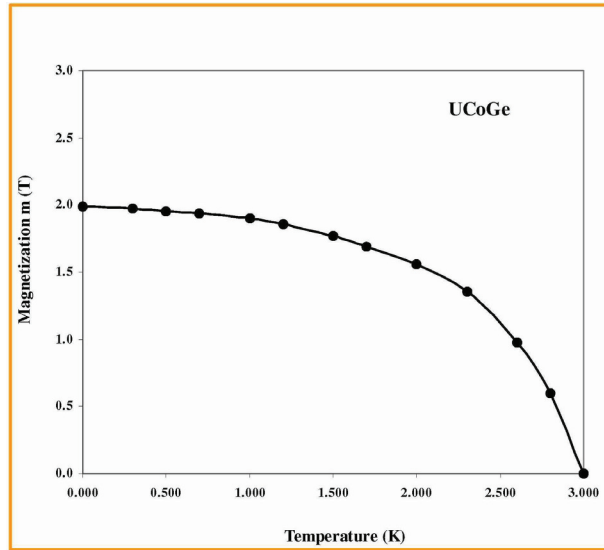


Figure 3: Variation of Magnetization with Temperature for UCoGe.

pair. This leads to a decrease in the superconducting gap (Δ) and hence T_c also reduces compared to the BCS value for given values of other relevant parameters. Obviously, increase in magnetization pushes the gap away from the Fermi surface and reduces its magnitude also. Our results agree with Karchev et al. [56] and Dahal et al. [57].

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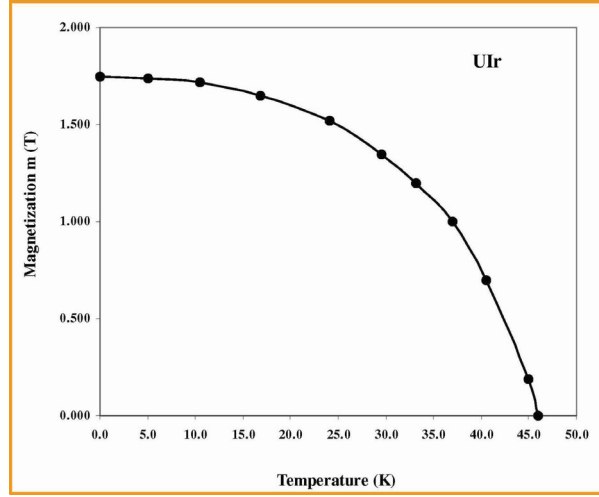


Figure 4: Variation of Magnetization (m) with Temperature for UIr.

Table 7: Order parameters (Δ , I) in the ferromagnetic, superconducting and ferromagnetic – superconducting coexistent states for UCoGe.

Temperature (T)				
K	Δ_{coex}	I_{coex}	I	Δ
0.00	1.90	2.20	0.40	0.25
0.20	1.89	2.15	0.46	0.16
0.40	1.87	1.90	0.50	0.12
0.60	1.85	1.13	0.40	0.16
0.80	1.80	0.24	0.00	0.26
0.85	1.78	0.00	-	-
1.00	1.72	-	-	-
1.20	1.63	-	-	-
1.40	1.52	-	-	-
1.60	1.40	-	-	-
1.80	1.24	-	-	-
2.00	1.05	-	-	-
2.20	0.85	-	-	-
2.40	0.65	-	-	-
2.60	0.45	-	-	-
3.00	0.00	-	-	-

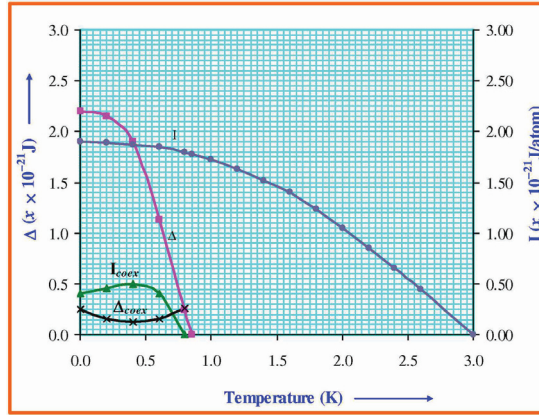


Figure 5: Order parameters of the ferromagnetic state ($\Delta = 0$, I), the superconducting state (Δ , $I = 0$) and the coexistence state ($\Delta \neq 0$, $I \neq 0$) as a function of temperature for UCoGe.

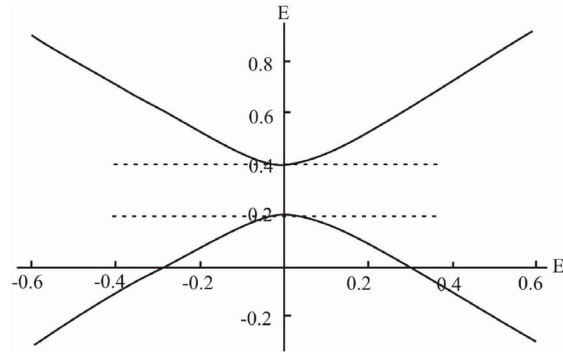


Figure 6: The energy spectrum of ferromagnetic superconductors. The upper curve corresponds to equation (30) and the lower one for equation (31). The upper horizontal line is at $U_m + \Delta$ and the lower horizontal line is at $U_m - \Delta$. The gap is 2Δ .

4.3 ENERGY SPECTRA AND DENSITY OF STATES

If we compare the quasi particle energy spectra (Equations (30) and (31)) with the BCS energy spectrum, $E = \sqrt{\epsilon_k^2 + \Delta^2}$, we see that the modification is due to the presence of ferromagnetic energy. The plot of energy spectrum is shown in fig. 6. It is very clear that the gap is not at the Fermi level, rather it is pushed up. Now, the energy spectrum is symmetric around U_m , contrary to the BCS case where it was symmetrical around $E = 0$.

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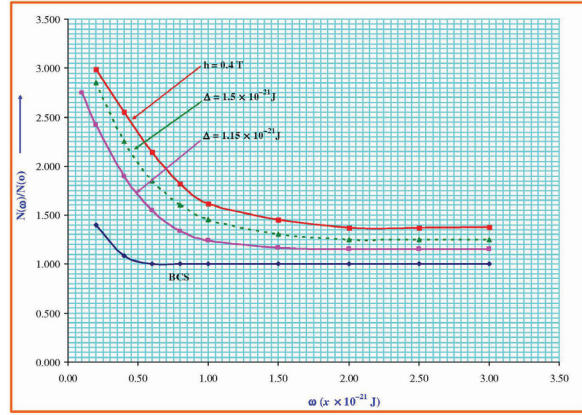


Figure 7: Density of States for UCoGe for $\Delta = 1.15 \times 10^{-21}\text{J}$ and $\Delta = 1.50 \times 10^{-21}\text{J}$.

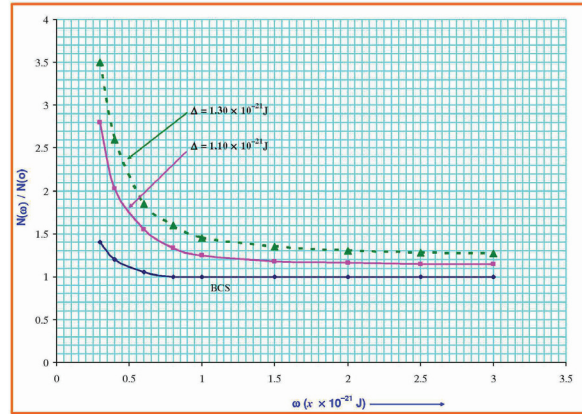


Figure 8: Variation of Density of states with ω for UIr for $\Delta = 1.10 \times 10^{-21}\text{J}$ and $\Delta = 1.30 \times 10^{-21}\text{J}$.

Expressions (40) and (41) converge to the density of states of the BCS model for $I = 0$ and $h = 0$, i.e.

$$\frac{N(\omega)}{N(0)} = \frac{|\omega|}{\sqrt{\omega^2 - \Delta^2}} \quad (\text{for } |\omega| > \Delta)$$

$$= 0 \quad (\text{for } |\omega| < 0)$$

Solving numerically equation (40) for UCoGe and UIr, we obtain the variation of $N(\omega)/N(0)$ with ω as shown in figures 7 and 8 respectively and corresponding

Table 8: Density of states for UCoGe

ω ($x \times 10^{-21}\text{J}$)	$N(\omega)/N(0)$			
	BCS	$\Delta = 1.15 \times 10^{-21}\text{J}$	$\Delta = 1.50 \times 10^{-21}\text{J}$	$h = 0.4\text{ T}$
0.10	-	2.75	-	-
0.20	1.400	2.42	2.85	2.99
0.40	1.087	1.90	2.25	2.55
0.60	1.000	1.55	1.85	2.14
0.80	1.000	1.34	1.60	1.82
1.00	1.000	1.24	1.45	1.62
1.50	1.000	1.17	1.30	1.45
2.00	1.000	1.15	1.25	1.37
2.50	1.000	1.15	1.25	1.37
3.00	1.000	1.15		1.38

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Table 9: Density of states for UIr

ω ($x \times 10^{-21}\text{J}$)	$N(\omega)/N(0)$		
	BCS	$\Delta = 1.10 \times 10^{-21}\text{J}$	$\Delta = 1.30 \times 10^{-21}\text{J}$
0.30	1.40	2.80	3.50
0.40	1.20	2.03	2.60
0.60	1.05	1.55	1.85
0.80	1.00	1.33	1.60
1.00	1.00	1.25	1.45
1.50	1.00	1.18	1.35
2.00	1.00	1.16	1.30
2.50	1.00	1.15	1.28
3.00	1.00	1.15	1.27

values are recorded in tables 8 and 9. We note that gap is pushed up (compared to BCS gap), giving rise to finite density at the Fermi level. Looking at the energy spectrum and density of states, one finds that the physical properties of the system will be dominated by the normal metal like behaviour. Our results agree with Dahal et al. [57], and Karchev et al. [56]. Small external field also pushes up Δ and in turn density of states rise at the Fermi level.

4.4 SPECIFIC HEAT

Solving numerically the expression (37) for specific heat divided by temperature (C/T) for UCoGe and UIr, values obtained are given in tables 10 and 11 and

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Table 10: Specific heat divided by temperature (C/T) for UCoGe

Temperature (T) K	C/T (mJ / mol – K ²)		
	BCS	Theory	Experimental
0.10	0.90	10	40.00
0.20	2.00	20	45.71
0.30	5.00	30	51.43
0.40	8.50	40	57.14
0.50	13.00	50	62.86
0.60	20.00	60	68.57
0.70	30.00	70	74.29
0.80	45.00	80	80.00
1.00	80.00	-	-

Table 11: Specific heat divided by temperature (C/T) for UIr

Temperature (T) K	C/T (mJ / mol – K ²)	
	Theory	BCS
0.02	8.45	0.90
0.04	16.90	2.50
0.06	25.35	5.20
0.08	33.80	10.00
0.10	42.25	16.50
0.12	50.70	26.00
0.14	60.00	40.20
0.16	-	60.00

variation of C/T versus T is obtained as shown in figures 9 and 10 respectively. From the graphs, we note:

- (i) A linear temperature dependence of C/T in coexistent state of ferromagnetism and superconductivity obtained from theory is in excellent agreement with experimental results for UCoGe [58] as opposed to the exponential decrease of specific heat in the BCS theory. Our results agree with Karchev et al. [56].
- (ii) Specific heat studies also confirm that T_c of ferromagnetic superconductors is affected by magnetic field, i.e. decreases slightly as compared to BCS value.

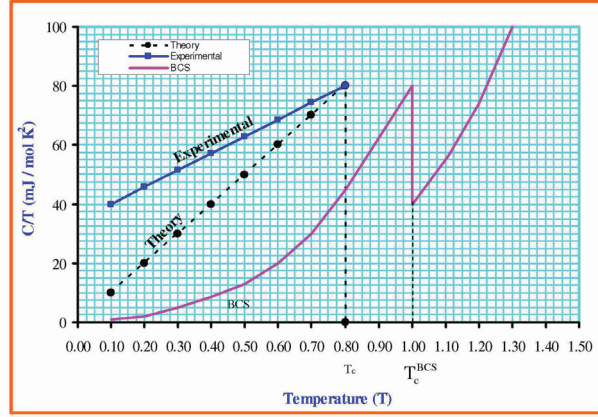


Figure 9: Variation of Electronic Specific heat divided by temperature (C/T) for UCoGe. Experimental curve [4] .

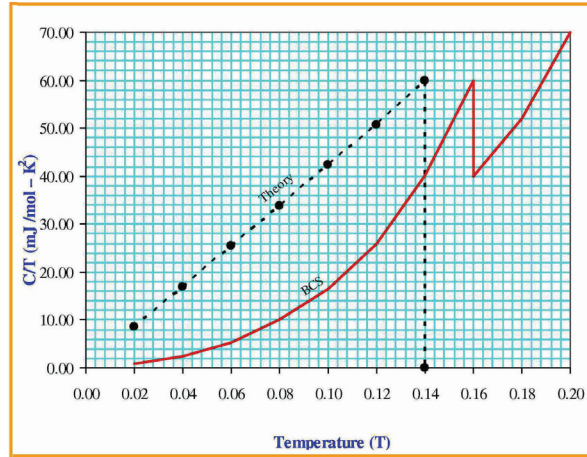


Figure 10: Variation of Electronic specific heat divided by temperature (C/T) for UIr.

4.5 FREE ENERGY AND CRITICAL FIELD

From equation (55), we note that

$$F_{FS} - F_{NF} \neq 0 \text{ and } \Delta^2 \neq 0$$

This clearly reveals that the phase transition from normal ferromagnetic state to superconducting -ferromagnetic state is first order phase transition [58].

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Table 12: Free energy difference ($F_{SF} - F_{NF}$) in the coexistent state for UCoGe

T/T_c	Free energy difference
	$-(F_{SF} - F_{NF})$
0.00	0.480
0.10	0.470
0.20	0.443
0.30	0.400
0.40	0.350
0.50	0.260
0.60	0.139
0.70	0.064
0.80	0.023
0.90	0.005
1.00	0.000

Table 13: Free energy difference ($F_{SF} - F_{NF}$) in the coexistent state for UIr

T/T_c	Free energy difference
	$-(F_{SF} - F_{NF})$
0.00	0.45
0.10	0.44
0.20	0.41
0.30	0.37
0.40	0.32
0.50	0.23
0.60	0.10
0.70	0.04
0.80	0.02
0.90	0.01
1.00	0.00

Expression (53) also shows that superconducting – ferromagnetic (SF) state has lower energy than the normal ferromagnetic (NF) state and therefore realized at low enough temperature. Our results agree with Karchev [56]. The free energy difference as function of temperature is shown in tables 12 and 13 and variation shown in figures 11 and 12 for UCoGe and UIr respectively. From these graphs, we note that the coexistent phase of

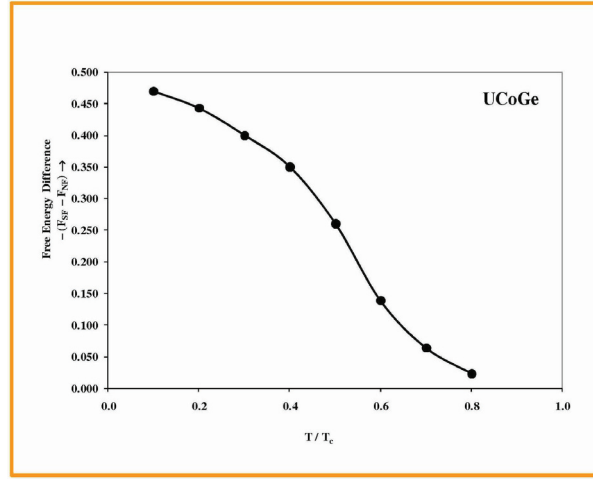


Figure 11: Free energy difference ($F_{SF} - F_{NF}$) as function of T/T_c for UCoGe, which displays coexistence of ferromagnetism and superconductivity below $T_c = 0.8$ K.

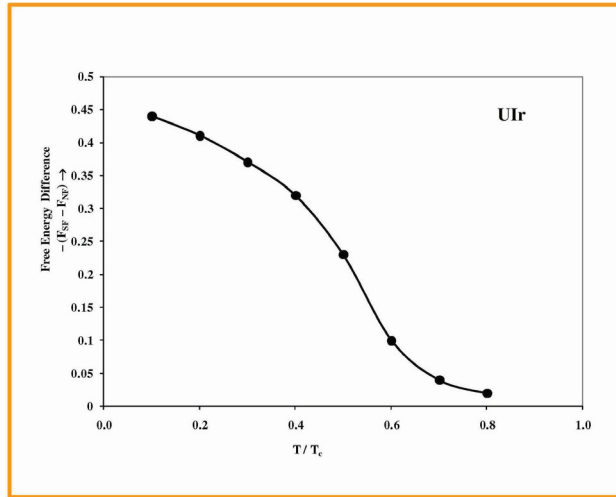


Figure 12: Free energy difference ($F_{SF} - F_{NF}$) as function of T/T_c for UIr, which displays coexistence of ferromagnetism and superconductivity below $T_c = 0.14$ K.

superconductivity and ferromagnetism is energetically favored compared to normal ferromagnetic case, which is consistent with the experimental fact that a transition to superconductivity – ferromagnetic state occurs well below the Curie temperature [4,59].

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Table 14: Critical Magnetic Field (H_c) for UCoGe

Temperature (T) K	Critical Magnetic Field (H_c (T))
0.00	1.600
0.10	1.590
0.20	1.523
0.30	1.413
0.40	1.232
0.50	0.950
0.60	0.616
0.70	0.300
0.80	0.000

Table 15: Critical Magnetic Field for UIr

Temperature (T) K	Critical Magnetic Field (H_c (T))
0.00	1.00
0.02	0.97
0.04	0.92
0.06	0.84
0.08	0.74
0.10	0.60
0.12	0.39
0.14	0.00

Variation of critical field with temperature obtained numerically by solving equation (57) is shown in table 14 and 15 for the systems UCoGe and UIr and variation is shown in figures 10 and 11 respectively. Critical field curves reveal that physical properties of the system are dominated by normal metal like behaviour.

5. CONCLUSIONS

In the BCS theory of superconductivity, the conduction electrons in a metal cannot be both ferromagnetically ordered and superconducting. Superconductors expel magnetic fields passing through them but strong magnetic fields kill the superconductivity. Even small amounts of magnetic impurities are usually enough to eliminate superconductivity. Much work has been done both theoretically and experimentally to understand the interplay

between ferromagnetism and superconductivity and to search for the possibility of true coexistence of these two ordered states. Prior to 2001, in all known ferromagnetic superconductors, the superconductivity phase is observed in a small part of the phase diagram. This situation has changed with the emergence of superconductivity under the background of ferromagnetic state in ZrZn_2 , UGe_2 , URhGe , UCoGe and UIr . In these ferromagnetic superconductors, a superconducting transition takes place at a temperature T_c deep in the ferromagnetic state, i.e. well below the Curie temperature T_{FM} , without expelling magnetic order. In uranium intermetallic compounds magnetism has a strong itinerant character and both ordering phenomena are carried by 5f electrons. Thus, it is proper to study a model where the coexistence of both ferromagnetism and superconductivity can be described by only one kind of electrons. Such a model study has recently been initiated by Karchev et al. [56].

We have studied the interplay between itinerant ferromagnetism and superconductivity in a model single – band homogeneous system by using a mean – field approximation. The superconducting part is treated by BCS theory and the itinerant ferromagnetic part is studied with the use of Hubbard Hamiltonian. Following Green's functions technique and equation of motion method, we have obtained coupled equations of superconducting gap (Δ) and magnetization (m). The two order parameters, m and Δ are coupled with each other through the distribution functions, which are also functions of m and Δ . We found that there are three nontrivial sets of solutions for Δ and m : the ferromagnetic ($\Delta = 0$, $m \neq 0$), the superconducting ($m = 0$, $\Delta \neq 0$), and the coexistent state ($\Delta \neq 0$ and $m \neq 0$).

We have closely studied the specific heat, energy spectra and density of states and free energy for a ferromagnetic superconductor considering that same electrons are responsible for both ordered states and superconductivity is due to s – wave pairing.

The specific heat has a linear temperature dependence ($C \propto T$) in the coexistence region as opposed to the exponential decrease of the specific heat in the BCS theory. Our result fits well the data observed experimentally for UCoGe . The specific heat has a linear temperature dependence as in the normal ferromagnetic metals, but increases anomalously at small magnetizations.

Free energy studies shows that the superconducting-ferromagnetic coexistence state has lower energy than normal ferromagnetic state and therefore coexistence state is realized at low enough temperature. Moreover, the ferromagnetic state never appears when the superconducting state is already in existence. This behaviour seems to be a particular feature of

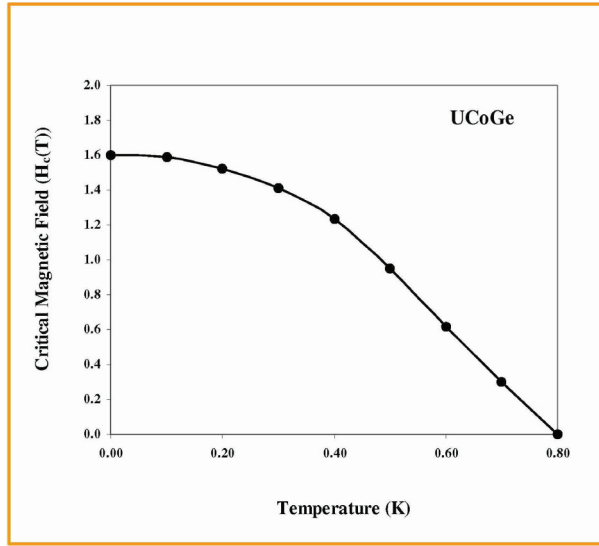


Figure 13: Variation of Critical Magnetic Field (H_c) with Temperature for UCoGe.

the itinerant π -electron model. For $T_c < T_{FM}$, there is a ferromagnetic to superconducting-ferromagnetic transition at $T = T_{coex} < T_c$, where T_{coex} is the temperature below which superconductivity and ferromagnetism coexist. For $T_{FM} < T_c$ and $T < T_c$, the superconducting state is more stable than the ferromagnetic state. This means that the ferromagnetic state can never be reentrant when the superconducting state is already present [10,60-63]. This is contrary to the situation in rare earth ternary compounds $ErRh_4B_4$ and $HoMo_6S_8$ [60,64], where superconductivity occurs at higher temperatures, and at lower temperatures the ferromagnetic state may appear.

This may be physically understood as follows: for localized ferromagnetism, the saturation magnetization, which depends on the magnitude of an individual local moment, and the Curie temperature, which depends on the exchange interaction between neighboring moments are not related to each other. The energy reduction due to the saturation magnetization may be quite large while the value of T_{FM} can be very small. For an itinerant system, the situation is quite different. Both the saturation magnetization and T_{FM} are decided dominantly by the Hubbard interaction U and the band structure. For a system with low T_{FM} , both the saturation magnetization and the energy reduction due to the magnetization will certainly be small. Therefore, when, $T_{FM} < T_c$, the itinerant ferromagnetic state is always at a disadvantage in energy as compared with the superconducting state.

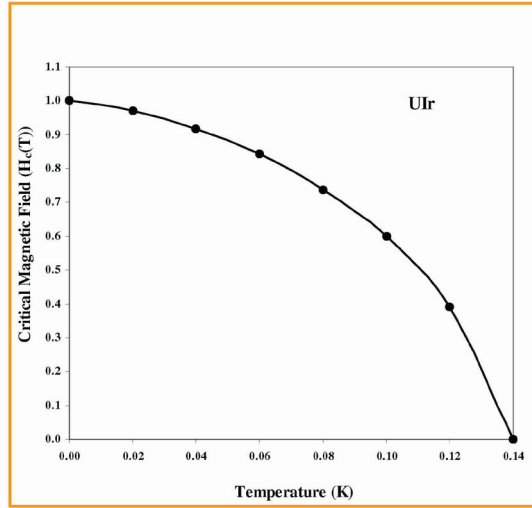


Figure 14: Variation of critical magnetic field (H_c) with Temperature (T) for UIr.

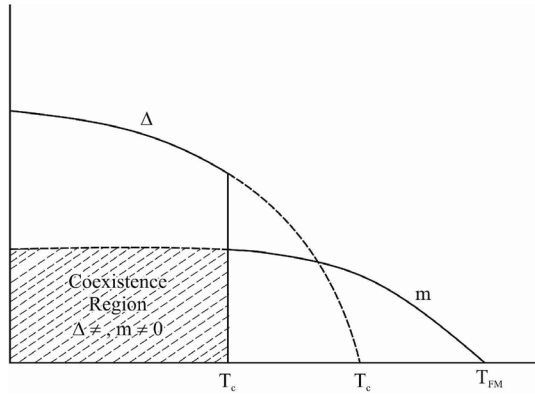


Figure 15: Phase diagram of itinerant ferromagnetic superconductors.

Blount and Varma [64] pointed that the electromagnetic coupling which results from the interaction between the superconducting d electrons and local magnetic moments of rare – earth ions plays a crucial role in ternary rare earth superconductors, ErRh_4B_4 and HoMo_6S_8 . For itinerant model, however, both the magnetism and superconductivity come from the electrons in the same f band. Here the main coupling is the Coulomb interaction between electrons, and the Hubbard model is an approximate description of this interaction. In our work, we have treated the magnetization as uniform and thus the electromagnetic coupling is absent.

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The study of the energy spectrum and the density of states reveals that the physical properties of the system are dominated by normal metal like behaviour.

The itinerant electron model developed by us provides a microscopic relationship between ferromagnetism and superconductivity. This model explains satisfactorily the behaviour of specific heat, energy spectra and density of states, free energy, etc. Our study unambiguously shows that superconductivity and itinerant ferromagnetism truly coexist in these systems and both ordering phenomena are carried by the same 5f electrons. Free energy study clearly reveals that it is possible to become superconducting via a first – order phase transition if the system on cooling first shows ferromagnetism. Our results are in agreement with Karchev [55], Linder and Sudbo [54] and Dahal et al. [57].

A possible phase diagram based on our model is as shown in fig.15.

It is well known that mean – field approximation has its limitation in treating ferromagnetism. We are not sure, whether and how an electromagnetic coupling or the coupling between superconducting electrons and magnetic fluctuations will be generated if the relevant part of the Coulomb interaction between f electrons is correctly taken into account . This question is certainly important and needs further investigation. For a more rigorous approach, the effect of magnetic fluctuations should also be considered. Since the mean – field theory is qualitatively correct away from T_{FM} , we expect that the essential features of our results should remain valid.

We hope in the near future measurements of the electronic and magnetic excitation spectra in the superconducting and magnetic phases of these systems will reveal crucial information on the superconducting gap structure and pairing mechanism. UCoGe may be the first material to reveal proof for the existence of the long – searched spontaneous vortex phase.

Progress in this field requires a new generation of pure crystals. Up to now, the attempts to discover Ce ferromagnetic superconductivity have failed.

With the discovery of weak itinerant ferromagnetic superconductors a new research theme in the field of magnetism and superconductivity has been disclosed. Research into ferromagnetic superconductors will help to unravel how magnetic fluctuations can stimulate superconductivity, which is a central theme running through materials families as diverse as the heavy fermion superconductors, high – T_c cuprates and recently discovered FeAs – based superconductors [65,66]. This novel insight might turn out to be crucial in the design of new superconducting materials.

An interesting aspect of ferromagnetic superconductivity concerns the influence of ferromagnetism on macroscopic phenomena such as Meissner effect [38]. Other related topics for further study are superconductivity in

ferromagnetic domain walls and the phenomena associated with the relative orientation of the superconducting order parameter to the magnetization, the effect of superconductivity on ferromagnetic domain structure [67], etc.

Theoretical Study
of Interplay
Between
Superconductivity
and Itinerant
Ferromagnetism

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